



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:30 PM UTC

PDB ID : 8CGZ / pdb_00008cgz
Title : tubulin-AB8939 complex
Authors : Varela, P.F.; Gigant, B.
Deposited on : 2023-02-06
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

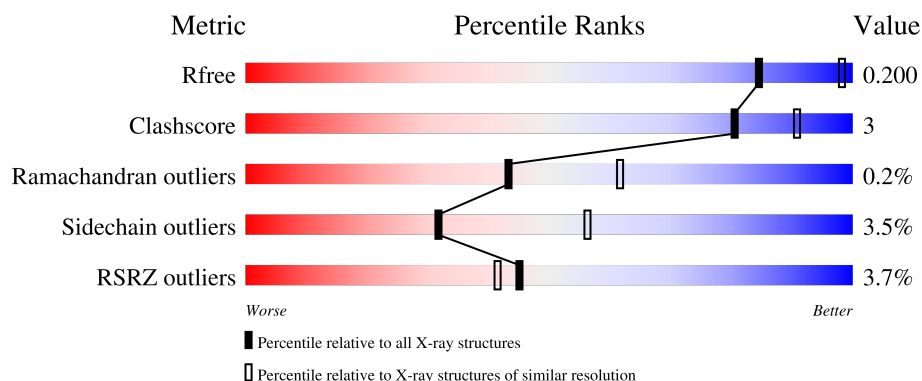
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	7% 86% 8% 5%
1	C	451	4% 87% 8% ...
2	B	445	2% 87% 8% ...
2	D	445	88% 7% ...
3	E	143	2% 73% 8% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14545 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3295	2085	562	626	22			
1	C	431	Total	C	N	O	S	0	0	0
			3359	2125	572	640	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	conflict	UNP D0VWZ0
A	340	SER	THR	conflict	UNP D0VWZ0
C	232	SER	GLY	conflict	UNP D0VWZ0
C	340	SER	THR	conflict	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

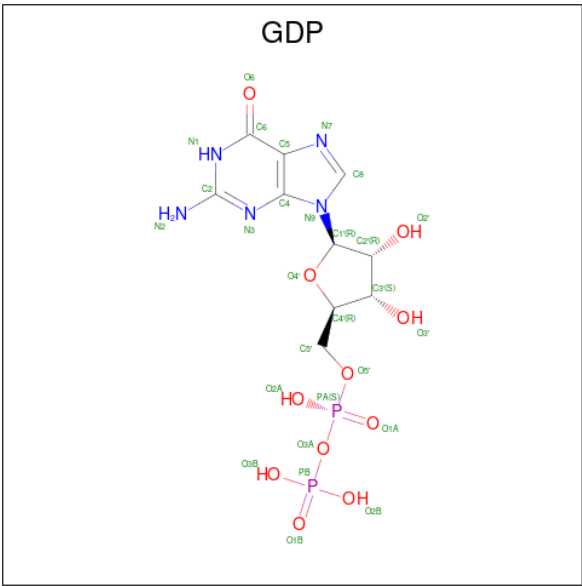
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3361	2109	576	649	27			
2	D	431	Total	C	N	O	S	0	0	0
			3375	2120	580	648	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	CYS	SER	conflict	UNP D0VWY9
B	318	ILE	VAL	conflict	UNP D0VWY9
D	203	CYS	SER	conflict	UNP D0VWY9
D	318	ILE	VAL	conflict	UNP D0VWY9

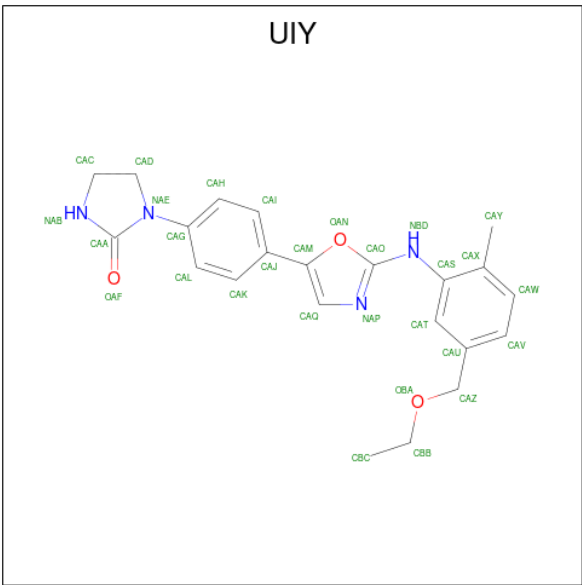
- Molecule 3 is a protein called Stathmin-4.

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 7 is AB-8939 (CCD ID: UIY) (formula: C₂₂H₂₄N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	4	3		
7	D	1	Total	C	N	O	0	0
			29	22	4	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is water.

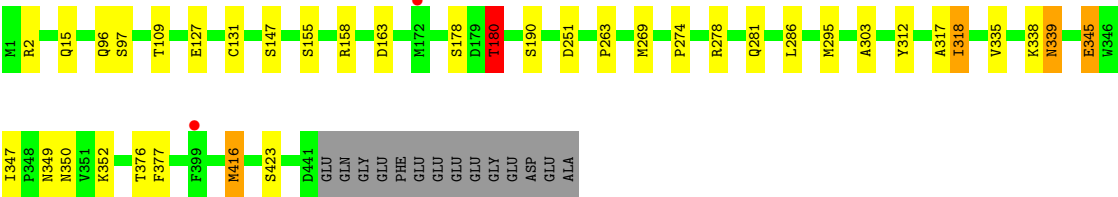
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	7	Total	O	0	0
			7	7		
9	C	21	Total	O	0	0
			21	21		
9	D	18	Total	O	0	0
			18	18		
9	E	1	Total	O	0	0
			1	1		

Chain D:

88%

7%

..



• Molecule 3: Stathmin-4

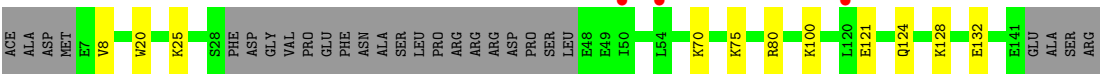
Chain E:

2%

73%

8%

19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.69Å 128.76Å 253.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.60 – 2.53 126.60 – 2.53	Depositor EDS
% Data completeness (in resolution range)	65.4 (126.60-2.53) 65.4 (126.60-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.52Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.197 , 0.235 0.201 , 0.200	Depositor DCC
R_{free} test set	2441 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14545	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UIY, SO4, GDP, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	1/3368 (0.0%)	1.00	3/4575 (0.1%)
1	C	0.72	0/3433	1.05	8/4660 (0.2%)
2	B	0.72	1/3434 (0.0%)	1.03	9/4652 (0.2%)
2	D	0.77	2/3450 (0.1%)	1.05	9/4674 (0.2%)
3	E	0.65	0/913	1.10	0/1220
All	All	0.72	4/14598 (0.0%)	1.04	29/19781 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	THR	CA-C	6.29	1.56	1.52
2	B	109	THR	CA-C	6.21	1.56	1.52
1	A	413	MET	SD-CE	-5.61	1.65	1.79
2	D	416	MET	SD-CE	5.18	1.92	1.79

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	ASP	CA-CB-CG	7.94	120.54	112.60
2	B	345	GLU	CB-CG-CD	7.12	124.71	112.60
2	B	96	GLN	CA-C-N	6.57	129.08	120.28
2	B	96	GLN	C-N-CA	6.57	129.08	120.28
2	D	96	GLN	CA-C-N	5.99	128.31	120.28
2	D	96	GLN	C-N-CA	5.99	128.31	120.28
2	D	163	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	338	LYS	CA-C-N	5.92	128.80	120.28
1	C	338	LYS	C-N-CA	5.92	128.80	120.28
2	D	97	SER	N-CA-C	5.86	117.66	111.28
2	B	97	SER	N-CA-C	5.76	117.56	111.28
2	D	345	GLU	CB-CG-CD	5.75	122.38	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	281	GLN	N-CA-C	5.65	117.42	108.67
1	C	62	VAL	N-CA-C	5.63	114.03	107.89
1	A	62	VAL	N-CA-C	5.60	113.99	107.89
2	D	180	THR	N-CA-CB	5.45	118.76	109.87
1	C	351	PHE	N-CA-C	5.42	118.32	109.59
2	D	251	ASP	CA-CB-CG	5.39	117.99	112.60
2	B	251	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	98	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	46	ASP	CA-C-N	5.28	131.63	121.54
1	C	46	ASP	C-N-CA	5.28	131.63	121.54
2	D	127	GLU	CB-CG-CD	5.12	121.30	112.60
2	D	180	THR	CB-CA-C	5.12	118.69	110.29
1	A	340	SER	CA-C-N	5.02	129.86	123.13
1	A	340	SER	C-N-CA	5.02	129.86	123.13
2	B	415	GLU	CA-C-N	5.02	127.00	120.28
2	B	415	GLU	C-N-CA	5.02	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3295	0	3166	21	0
1	C	3359	0	3266	18	0
2	B	3361	0	3240	19	0
2	D	3375	0	3254	16	0
3	E	905	0	876	6	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	0	0
6	D	28	0	12	0	0
7	B	29	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	29	0	0	1	0
8	B	10	0	0	0	0
8	D	5	0	0	1	0
9	A	8	0	0	0	0
9	B	7	0	0	0	0
9	C	21	0	0	0	0
9	D	18	0	0	0	0
9	E	1	0	0	0	0
All	All	14545	0	13850	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:124:GLN:HB3	3:E:128:LYS:HZ2	1.38	0.88
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.65	0.78
1:A:103:TYR:HD1	1:A:413:MET:HE1	1.53	0.73
3:E:124:GLN:HB3	3:E:128:LYS:NZ	2.03	0.72
2:B:345:GLU:HG3	2:B:440:ALA:HB2	1.71	0.70
1:C:121:ARG:HD3	1:C:124:LYS:NZ	2.08	0.69
1:A:121:ARG:HD3	1:A:124:LYS:NZ	2.08	0.69
3:E:124:GLN:C	3:E:128:LYS:HZ2	2.07	0.62
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.81	0.62
3:E:124:GLN:CB	3:E:128:LYS:HZ2	2.12	0.62
1:A:103:TYR:CD1	1:A:413:MET:HE1	2.36	0.60
2:B:281:GLN:H	2:B:281:GLN:CD	2.10	0.59
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.86	0.58
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.86	0.58
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.36	0.54
2:D:318:ILE:HG23	2:D:376:THR:HB	1.91	0.53
3:E:8:VAL:HG13	3:E:20:TRP:CD1	2.43	0.53
2:B:345:GLU:CG	2:B:440:ALA:HB2	2.39	0.53
1:A:221:ARG:HD3	2:B:325:MET:HE3	1.91	0.53
2:D:295:MET:HE3	2:D:377:PHE:HD2	1.74	0.52
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.91	0.52
2:D:295:MET:HE1	2:D:317:ALA:CB	2.39	0.51
1:A:121:ARG:HA	1:A:124:LYS:HE2	1.93	0.50
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.93	0.50
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:HA	1:C:124:LYS:HE2	1.93	0.49
1:A:121:ARG:HD3	1:A:124:LYS:HZ3	1.74	0.49
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.93	0.49
1:C:96:LYS:HE3	2:D:131:CYS:HB2	1.94	0.49
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.48	0.49
2:D:295:MET:HE1	2:D:317:ALA:HB2	1.94	0.48
1:C:250:VAL:HG13	1:C:254:GLU:HB3	1.94	0.48
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.94	0.48
1:A:104:ALA:CB	1:A:413:MET:HE3	2.40	0.48
2:D:338:LYS:C	2:D:339:ASN:HD22	2.23	0.47
1:C:359:PRO:HB2	1:C:370:LYS:NZ	2.30	0.47
1:C:121:ARG:CD	1:C:124:LYS:NZ	2.77	0.47
1:A:359:PRO:HB2	1:A:370:LYS:NZ	2.29	0.46
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.96	0.46
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.98	0.46
1:A:121:ARG:CD	1:A:124:LYS:NZ	2.76	0.46
3:E:124:GLN:C	3:E:128:LYS:NZ	2.74	0.45
2:B:338:LYS:C	2:B:339:ASN:HD22	2.23	0.45
1:C:339:ARG:NH1	1:C:340:SER:OG	2.50	0.45
2:D:147:SER:HB2	2:D:190:SER:OG	2.16	0.45
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.53	0.44
2:B:164:ARG:HA	2:B:164:ARG:HE	1.83	0.44
1:C:121:ARG:CD	1:C:124:LYS:HZ1	2.31	0.44
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.52	0.44
2:B:416:MET:HE2	2:B:416:MET:HB2	1.88	0.44
2:B:281:GLN:CD	2:B:281:GLN:N	2.76	0.43
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.36	0.43
2:D:416:MET:HE2	2:D:416:MET:HB2	1.92	0.43
2:B:181:VAL:CG1	1:C:350:GLY:HA2	2.49	0.43
1:C:133:GLN:HB3	1:C:252:LEU:HD12	1.99	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.54	0.43
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.00	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.42
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.37	0.42
2:D:278:ARG:NH2	8:D:503:SO4:O2	2.51	0.42
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.02	0.42
1:A:71:GLU:HB3	1:A:98:ASP:HB3	2.02	0.42
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.02	0.41
1:C:121:ARG:HD3	1:C:124:LYS:HZ1	1.83	0.41
1:C:121:ARG:HD3	1:C:124:LYS:HZ3	1.82	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:SER:OG	2:D:180:THR:HG23	2.21	0.41
1:C:192:HIS:CG	1:C:421:ALA:HA	2.56	0.41
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.08	0.41
2:B:352:LYS:HD2	7:B:502:UIY:CAL	2.51	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.56	0.41
2:B:101:ASN:HB2	2:B:180:THR:HG21	2.03	0.40
2:D:352:LYS:HD2	7:D:502:UIY:CAH	2.51	0.40
2:B:308:ARG:NH2	2:B:339:ASN:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/451 (93%)	411 (98%)	8 (2%)	2 (0%)	24	41
1	C	427/451 (95%)	415 (97%)	10 (2%)	2 (0%)	24	41
2	B	428/445 (96%)	417 (97%)	11 (3%)	0	100	100
2	D	429/445 (96%)	422 (98%)	7 (2%)	0	100	100
3	E	112/143 (78%)	110 (98%)	2 (2%)	0	100	100
All	All	1817/1935 (94%)	1775 (98%)	38 (2%)	4 (0%)	43	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	C	350	GLY
1	A	131	GLY
1	C	131	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/379 (92%)	340 (98%)	8 (2%)	44	70
1	C	361/379 (95%)	350 (97%)	11 (3%)	36	62
2	B	367/383 (96%)	351 (96%)	16 (4%)	25	47
2	D	368/383 (96%)	356 (97%)	12 (3%)	33	58
3	E	88/125 (70%)	81 (92%)	7 (8%)	11	22
All	All	1532/1649 (93%)	1478 (96%)	54 (4%)	32	56

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	GLU
1	A	88	HIS
1	A	178	SER
1	A	196	GLU
1	A	315	CYS
1	A	318	LEU
1	A	358	GLN
2	B	2	ARG
2	B	15	GLN
2	B	39	ASP
2	B	155	SER
2	B	164	ARG
2	B	180	THR
2	B	238	VAL
2	B	247	GLN
2	B	281	GLN
2	B	298	SER
2	B	318	ILE
2	B	325	MET
2	B	335	VAL
2	B	339	ASN
2	B	405	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	423	SER
1	C	71	GLU
1	C	123	ARG
1	C	164	LYS
1	C	178	SER
1	C	241	SER
1	C	279	GLU
1	C	280	LYS
1	C	315	CYS
1	C	318	LEU
1	C	339	ARG
1	C	340	SER
2	D	2	ARG
2	D	15	GLN
2	D	155	SER
2	D	158	ARG
2	D	180	THR
2	D	281	GLN
2	D	318	ILE
2	D	335	VAL
2	D	339	ASN
2	D	345	GLU
2	D	349	ASN
2	D	423	SER
3	E	25	LYS
3	E	70	LYS
3	E	75	LYS
3	E	80	ARG
3	E	100	LYS
3	E	121	GLU
3	E	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	285	GLN
1	A	309	HIS
1	A	372	GLN
1	A	393	HIS
2	B	8	GLN
2	B	11	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	14	ASN
2	B	15	GLN
2	B	59	ASN
2	B	136	GLN
2	B	331	GLN
2	B	349	ASN
1	C	61	HIS
1	C	293	ASN
1	C	372	GLN
1	C	393	HIS
2	D	11	GLN
2	D	15	GLN
2	D	59	ASN
2	D	331	GLN
3	E	108	ASN
3	E	136	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	D	503	-	4,4,4	0.35	0	6,6,6	0.49	0
6	GDP	B	501	-	29,30,30	0.33	0	45,47,47	0.54	0
7	UIY	D	502	-	32,32,32	1.46	5 (15%)	41,44,44	1.36	4 (9%)
8	SO4	B	503	-	4,4,4	0.43	0	6,6,6	0.22	0
4	GTP	C	600	5	33,34,34	0.47	0	50,54,54	0.58	0
4	GTP	A	600	5	33,34,34	0.41	0	50,54,54	0.58	1 (2%)
6	GDP	D	501	-	29,30,30	0.39	0	45,47,47	0.64	1 (2%)
8	SO4	B	504	-	4,4,4	0.31	0	6,6,6	0.11	0
7	UIY	B	502	-	32,32,32	1.76	4 (12%)	41,44,44	1.83	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	B	501	-	-	6/16/32/32	0/3/3/3
7	UIY	D	502	-	-	2/16/26/26	0/4/4/4
4	GTP	C	600	5	-	8/22/38/38	0/3/3/3
4	GTP	A	600	5	-	9/22/38/38	0/3/3/3
6	GDP	D	501	-	-	6/16/32/32	0/3/3/3
7	UIY	B	502	-	-	0/16/26/26	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	UIY	CAA-NAE	7.87	1.44	1.38
7	D	502	UIY	CAA-NAE	4.90	1.42	1.38
7	D	502	UIY	CAQ-CAM	2.53	1.38	1.34
7	B	502	UIY	CAA-NAB	2.30	1.41	1.34
7	D	502	UIY	CAT-CAU	2.28	1.43	1.39
7	D	502	UIY	CAO-NAP	2.20	1.39	1.33
7	B	502	UIY	CAQ-NAP	2.18	1.41	1.37
7	D	502	UIY	CAT-CAS	2.05	1.42	1.39
7	B	502	UIY	CAV-CAU	-2.03	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	UIY	OAF-CAA-NAE	5.22	129.90	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	UIY	OAF-CAA-NAE	4.40	129.25	125.82
7	B	502	UIY	NAB-CAA-NAE	-3.95	104.60	107.43
7	B	502	UIY	CAI-CAJ-CAM	-3.84	114.67	120.77
7	B	502	UIY	CAC-CAD-NAE	-3.49	99.46	103.05
7	B	502	UIY	CAC-NAB-CAA	-3.18	110.39	113.58
7	B	502	UIY	CAK-CAJ-CAM	2.67	125.00	120.77
7	D	502	UIY	CAY-CAX-CAS	2.53	124.10	121.23
7	D	502	UIY	OBA-CAZ-CAU	-2.39	103.28	110.77
7	B	502	UIY	CAT-CAS-CAX	-2.21	117.14	119.75
6	D	501	GDP	O3B-PB-O3A	2.20	112.02	104.64
7	D	502	UIY	NAB-CAA-NAE	-2.17	105.87	107.43
4	A	600	GTP	O5'-PA-O1A	2.13	117.36	108.94

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	PB-O3B-PG-O2G
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O1A
7	D	502	UIY	CAU-CAZ-OBA-CBB
4	A	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
6	B	501	GDP	PB-O3A-PA-O2A
6	D	501	GDP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	C3'-C4'-C5'-O5'
7	D	502	UIY	NAP-CAO-NBD-CAS
4	C	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	O4'-C4'-C5'-O5'
4	C	600	GTP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

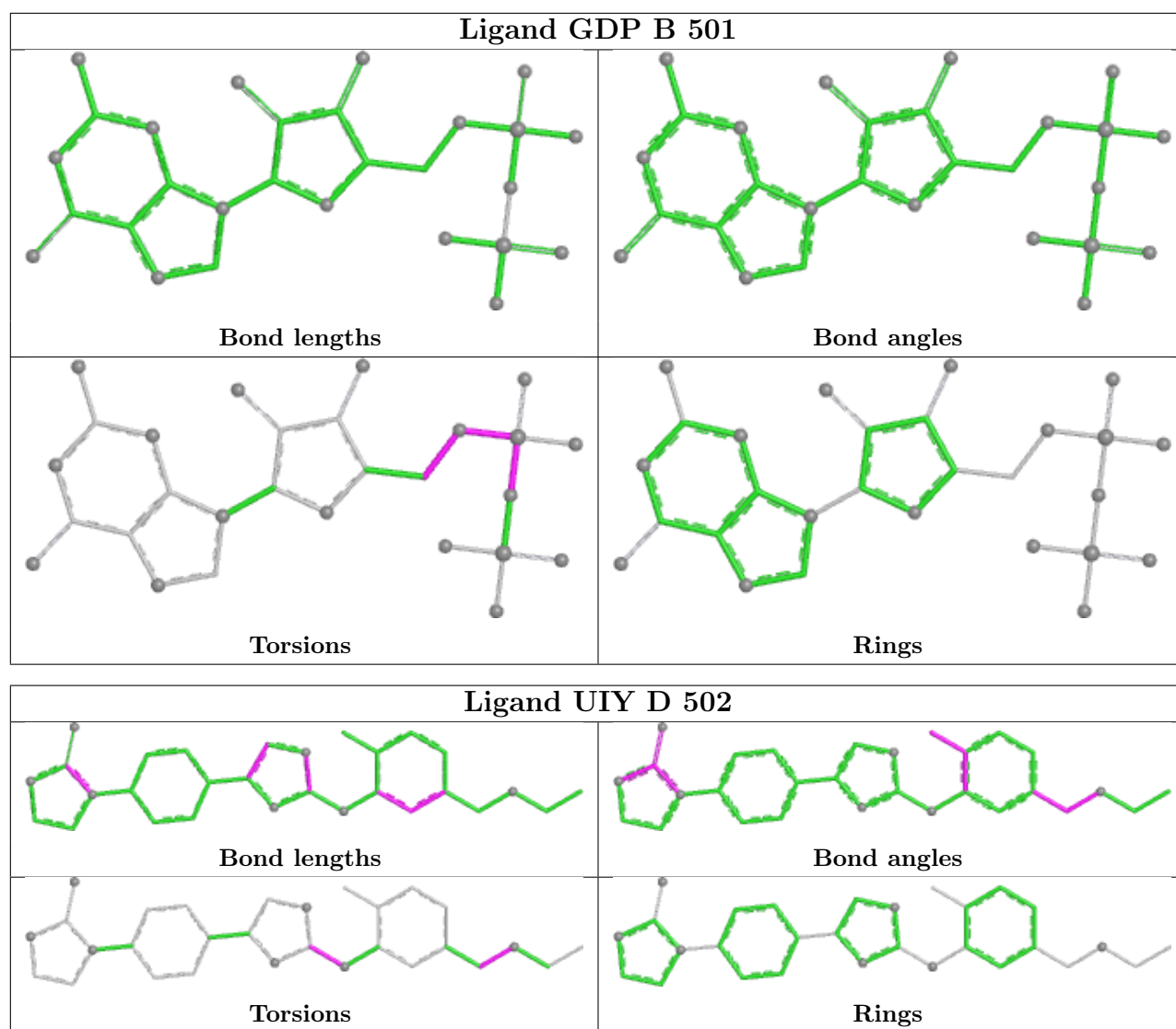
Mol	Chain	Res	Type	Atoms
6	B	501	GDP	PB-O3A-PA-O1A
6	D	501	GDP	PB-O3A-PA-O1A
6	B	501	GDP	C4'-C5'-O5'-PA
6	D	501	GDP	C4'-C5'-O5'-PA
4	A	600	GTP	C4'-C5'-O5'-PA
4	A	600	GTP	PB-O3A-PA-O1A

There are no ring outliers.

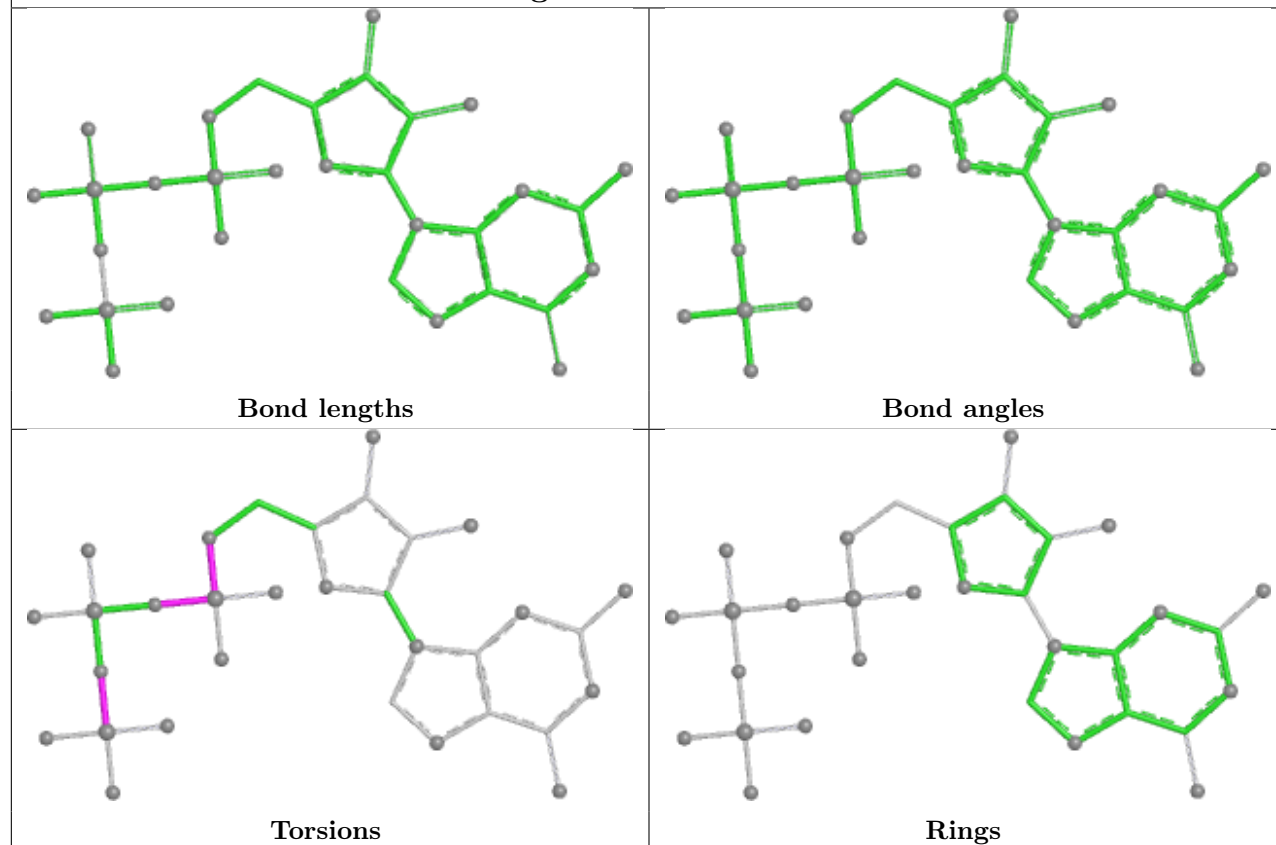
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	503	SO4	1	0
7	D	502	UIY	1	0
7	B	502	UIY	1	0

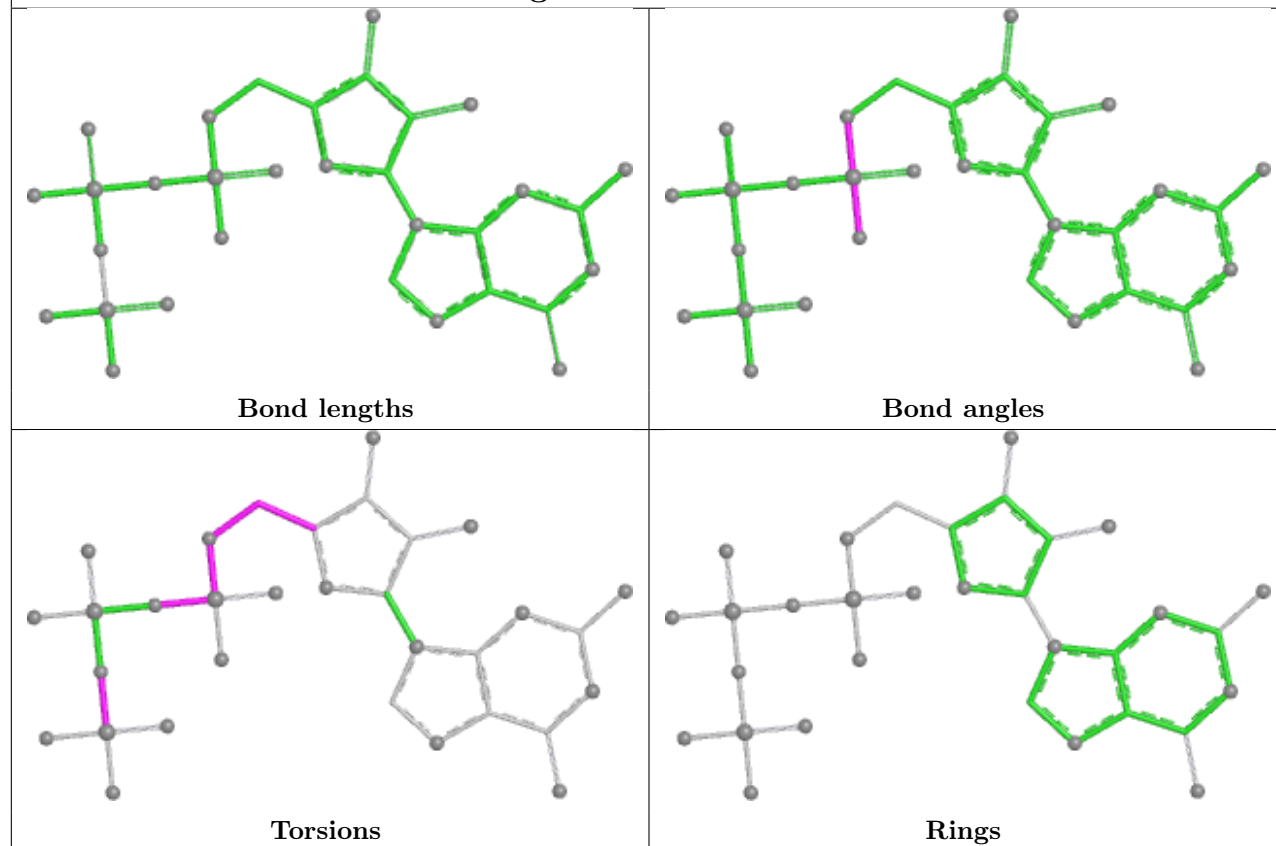
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

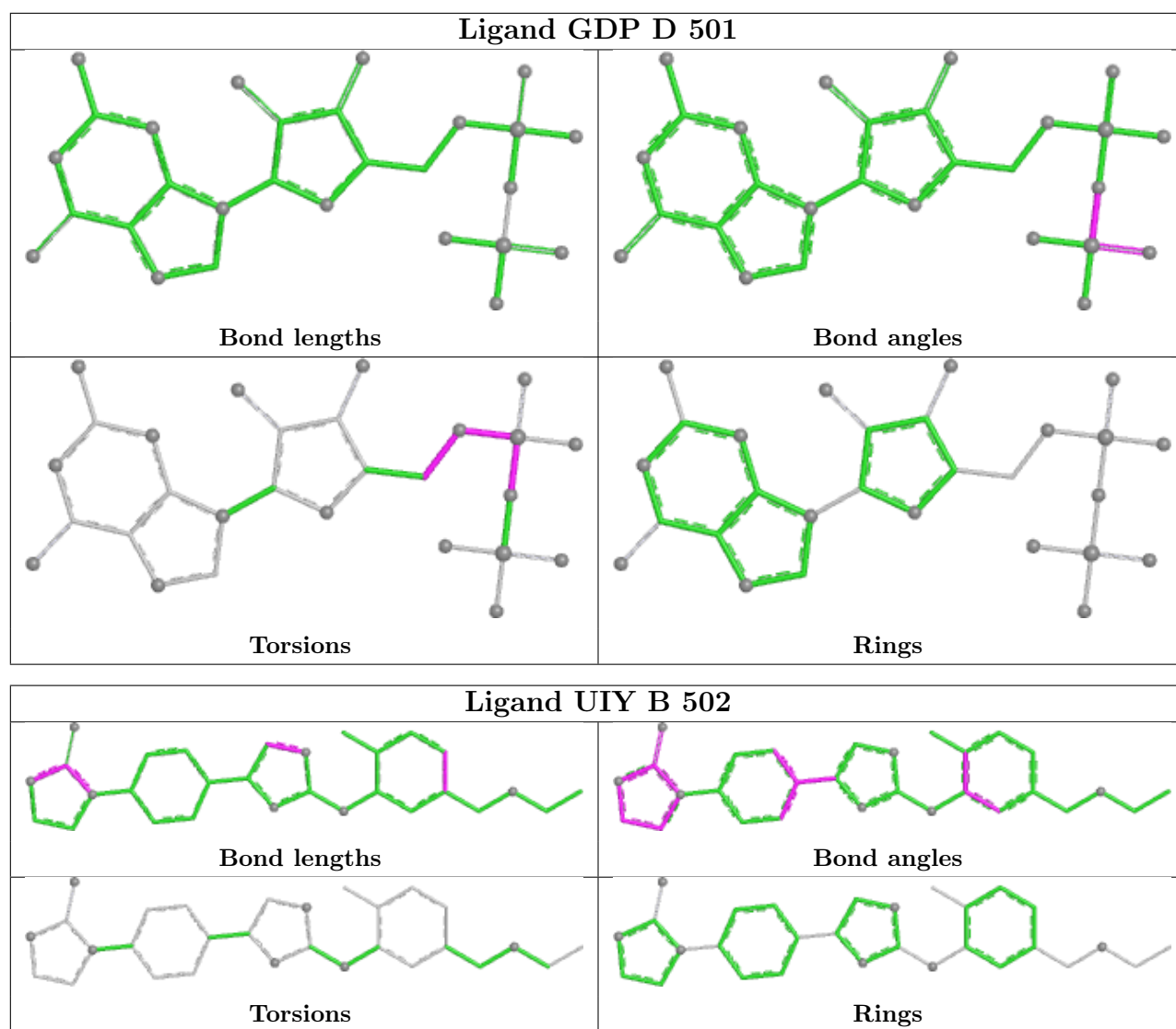


Ligand GTP C 600



Ligand GTP A 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/451 (94%)	0.56	33 (7%) 19 17	68, 105, 149, 167	0
1	C	431/451 (95%)	0.43	18 (4%) 40 37	52, 92, 136, 155	0
2	B	430/445 (96%)	0.30	11 (2%) 57 53	59, 86, 126, 143	0
2	D	431/445 (96%)	0.18	2 (0%) 87 85	49, 75, 116, 131	0
3	E	116/143 (81%)	0.69	3 (2%) 57 53	102, 123, 162, 169	0
All	All	1835/1935 (94%)	0.39	67 (3%) 45 41	49, 92, 138, 169	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	CYS	5.8
1	C	68	VAL	4.4
1	C	37	PRO	4.0
1	A	376	CYS	3.7
1	A	318	LEU	3.6
1	C	315	CYS	3.6
2	B	295	MET	3.5
1	A	234	ILE	3.4
2	B	181	VAL	3.4
2	D	172	MET	3.4
1	A	378	LEU	3.4
1	A	57	GLY	3.4
3	E	50	ILE	3.4
1	A	319	TYR	3.3
1	C	313	MET	3.2
1	C	65	ALA	3.1
3	E	54	LEU	3.1
1	A	328	VAL	3.0
1	A	351	PHE	2.9
1	A	313	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	122	ILE	2.8
1	A	122	ILE	2.8
1	C	302	MET	2.8
1	A	315	CYS	2.8
1	C	350	GLY	2.7
1	A	283	HIS	2.7
1	C	7	ILE	2.7
2	B	400	ARG	2.7
1	C	135	PHE	2.7
2	B	296	PHE	2.7
1	A	259	LEU	2.6
1	A	332	ILE	2.6
1	A	337	THR	2.5
2	B	241	CYS	2.5
1	C	169	PHE	2.5
1	A	437	VAL	2.5
1	A	302	MET	2.5
2	B	126	SER	2.5
1	A	323	VAL	2.4
1	C	346	TRP	2.4
2	B	177	VAL	2.4
1	A	317	LEU	2.4
2	B	291	LEU	2.4
1	A	341	ILE	2.3
1	C	136	LEU	2.3
1	A	46	ASP	2.3
1	C	281	ALA	2.3
2	B	213	CYS	2.3
1	A	227	LEU	2.2
1	A	203	MET	2.2
1	A	56	THR	2.2
1	A	4	CYS	2.2
1	A	58	ALA	2.1
2	B	435	TYR	2.1
1	A	335	ILE	2.1
1	A	308	ARG	2.1
1	A	307	PRO	2.1
1	C	16	ILE	2.1
1	A	38	SER	2.1
1	C	66	VAL	2.1
1	C	137	VAL	2.0
3	E	120	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	384	ILE	2.0
1	A	295	CYS	2.0
2	D	399	PHE	2.0
1	A	367	ASP	2.0
2	B	172	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

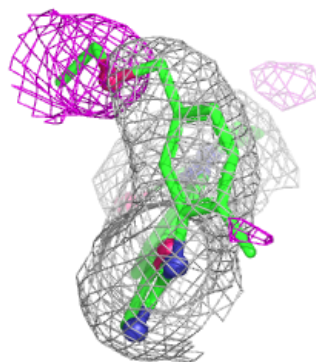
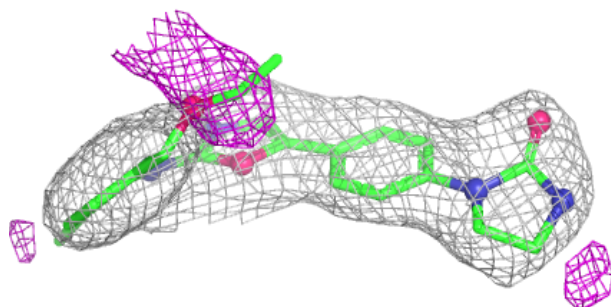
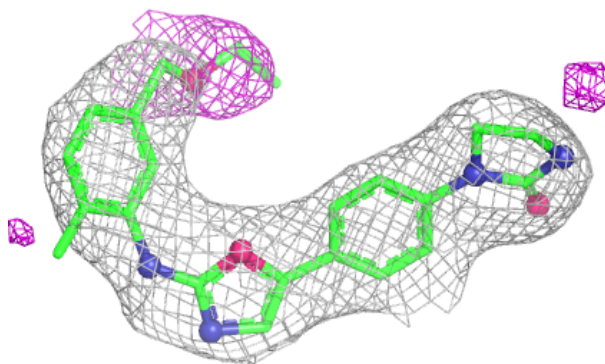
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	B	503	5/5	0.70	0.08	142,142,142,142	0
8	SO4	B	504	5/5	0.74	0.08	175,175,175,175	0
8	SO4	D	503	5/5	0.88	0.10	148,148,148,149	0
7	UIY	B	502	29/29	0.94	0.11	72,73,81,81	0
7	UIY	D	502	29/29	0.95	0.09	59,60,63,64	0
6	GDP	B	501	28/28	0.95	0.07	76,78,81,81	0
6	GDP	D	501	28/28	0.96	0.07	56,63,70,71	0
5	MG	C	601	1/1	0.96	0.10	59,59,59,59	0
4	GTP	A	600	32/32	0.97	0.07	68,71,73,73	0
4	GTP	C	600	32/32	0.97	0.07	65,67,68,69	0
5	MG	A	601	1/1	0.99	0.07	73,73,73,73	0

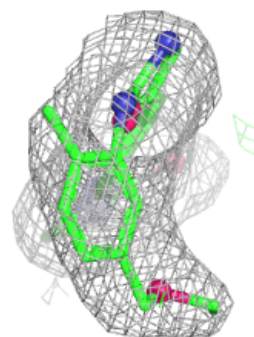
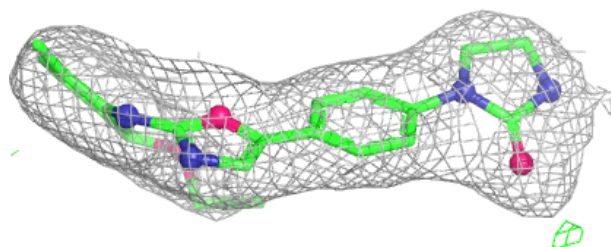
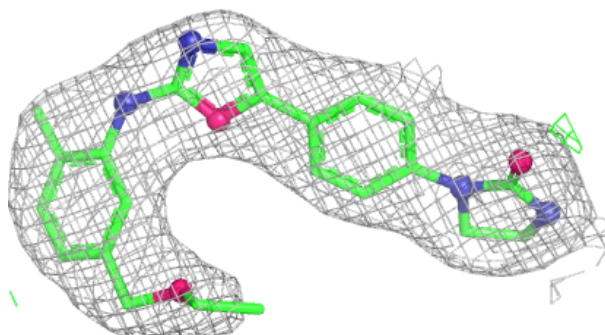
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UIY B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

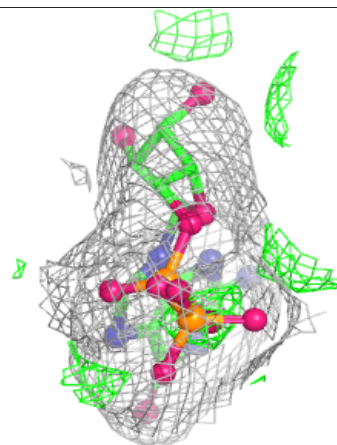
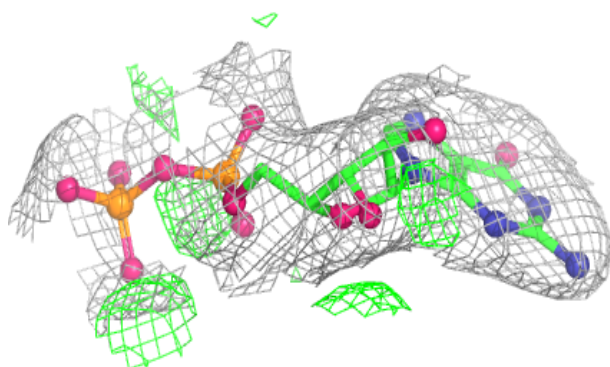
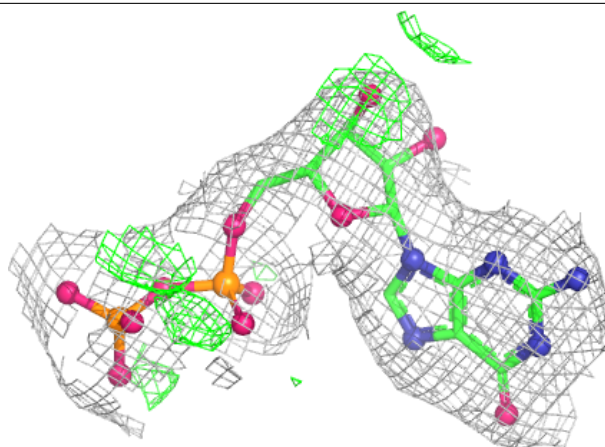
**Electron density around UIY D 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

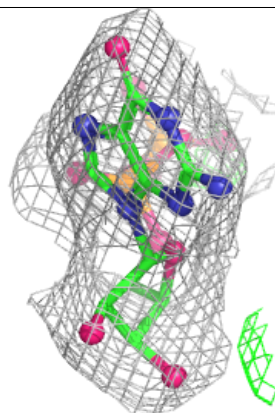
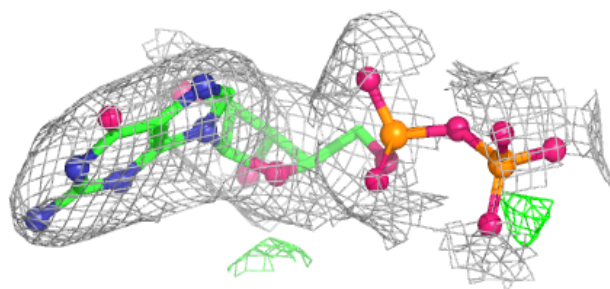
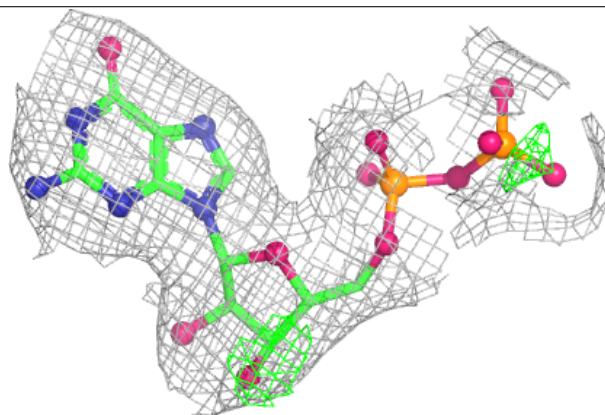


Electron density around GDP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

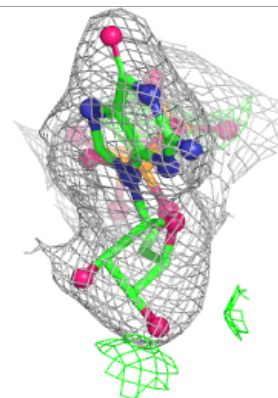
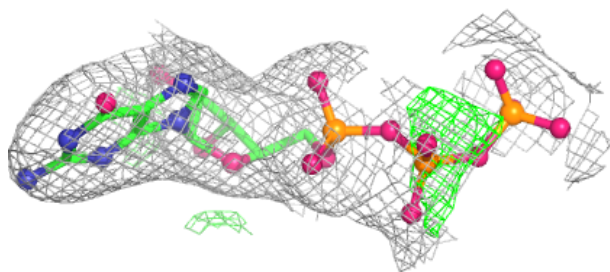
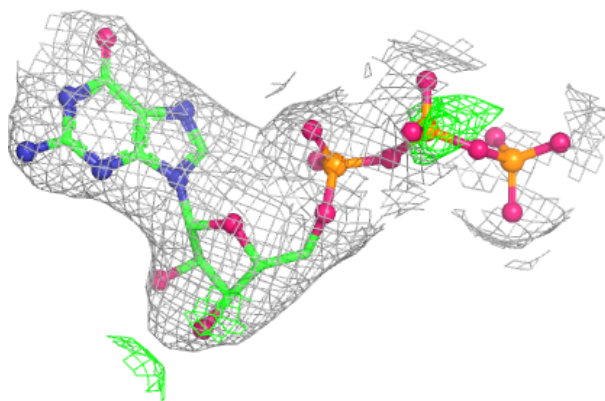
**Electron density around GDP D 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

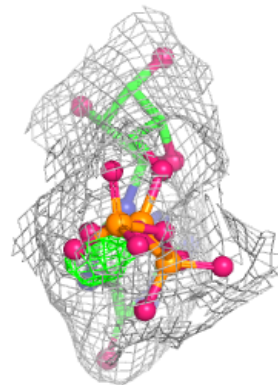
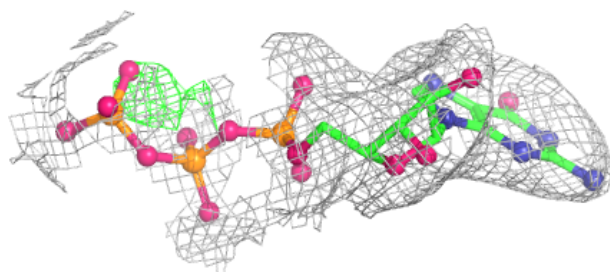
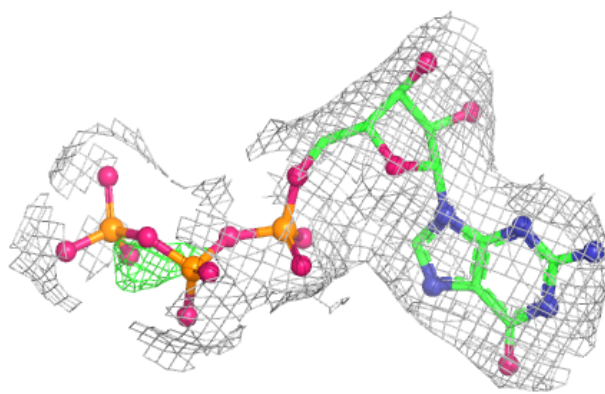


Electron density around GTP A 600:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GTP C 600:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.